ID: P2.13

Title: Thermodynamics of Energy Conversion Devices

Name: Rogers, David

Affiliation: Sandia National Laboratories

We present a novel framework for analyzing dynamic processes arbitrarily far from thermal equilibrium. This is made possible by a combination of two extremum principles: Hamilton's principle of stationary action and Gibbs' principle of maximum entropy. Application to particle motion gives the Langevin and Brownian equations. Application to Hamiltonian fluid dynamics gives the Navier-Stokes equations. The origin of the theory in maximum entropy methods allows important parallels to be drawn to the usual equilibrium statistical mechanics. One such result is the derivation of Green-Kubo relations for transient fluctuations as simple Maxwell-Gibbs relations. An application to ion channel kinetics is presented to show the validity of this theorem. Another important result is the existence of a microscopic form of the second law that includes effects from heat and work exchange with the external environment plus a novel contribution from the information entropy of the system. This result is applied to analyze entropy production in an optical bead pulling experiment, identifying an interpretation for the information entropy as work of compression. Other applications to transition path sampling computations and their energetic decompositions for ion-protein interaction will be discussed if time permits. This work was supported, in part, by Sandia's LDRD program, and, in part, by the National Institutes of Health through the NIH Road Map for Medical Research. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.